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14. ABSTRACT
This brief report covers studies of the stability of a well-characterized model of a metal-metalloid glassy alloy (A3B) in contact with a planar surface of a stable congruent crystal (i.e., crystal with the same composition as the glass) through computer simulations based on a NPT symplectic algorithm based on Nose-Hoover constraints developed recently by Laird.

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Project: Stability and Structure of the Interface between a Metallic Glass and its Congruent Crystal Phases

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A long standing question about the structure of amorphous metallic alloys concerns the role played by domains of crystalline order – either the stable crystal phase or metastable polytopes. There has been little progress in clarifying this issue because of the difficulty in identifying often distorted crystalline domains and the lack of any satisfactory method of establishing the degree to which a given structure contributes to the stability of the phase. In this project we are addressing these problems by considering the structure and stability of the glass-crystal interface. Drawing on the work of Köster on the crystallization kinetics we have identified a number of possible forms that the glass-crystal interface may take. These are a) a 'conventional' interface consisting of a continuous transition between melt and crystal, b) an interface in which a substitionally disordered crystal structure intercedes between the melt and the crystal, and c) an interface in which a metastable or quasicrystalline structure intercedes between the melt and crystal.

We are studying the stability of a well characterized model of a metal-metalloid glassy alloy in contact with a planar surface of a stable congruent crystal (i.e crystal with the same composition as the glass) through computer simulations. We have extensively characterized the stability of an A_3B alloy, initially introduced as a model for NiP. We have also established the stability of two A_3B crystals for this model: the Ni_3P and the Fe_3C structures. We have established that the melting points of both of these crystals are considerably higher than the temperature below which we can no longer observe structural relaxation and self diffusion (i.e the computer 'glass transition temperature'). This is an important feature of the calculations since it ensures that we are working at temperatures at which either crystal growth or just relaxation of the interfacial structure can take place on accessible time scales.

The simulations are being carried out at constant pressure and temperature over a range of compositions using a constant NPT symplectic algorithm based on Nose-Hoover constraints developed recently by Laird. This algorithm allows for longer time steps than higher order methods. We can carry out runs of up to 10^7 time steps, the equivalent of roughly 10 nanoseconds. While this time is obviously short in comparison to experimental time scales, two points should be kept in mind when considering the physical relevance of such short simulations. First, 10^7 time steps is typically between 10 and 100 times the structural relaxation time over the temperature ranges we study. This means that we are able to study the development of glass-like phenomena in well characterised metastable equilibrium states. Second, we can complete accurate 'measurements' of structural and kinetic properties well within the run times. This is roughly 10^9 times faster than these measurements can be carried out experimentally

(assuming 10s for an experimental measurement). As a result, simulations do not need to stabilise amorphous states as long as experiments in order to be able to properly characterise them.

Currently we are establishing the conditions which will result in crystallization and those which will result in a stationary crystal-glass interface. This process has proved time consuming due to the slow dynamics associated with this interface, making it difficult to distinguish between growth and relaxation without performing very long simulation runs. We are particularly excited at the prospect of studying the collective fluctuations associated with crystallization of a glass-forming alloy, especially as the crystal structures are considerably more complex than any whose growth has been simulated to date. We are also calculating the variation of the atomic mobility through the interfacial region as there have been suggestions that the glass-crystal interface may exhibit enhanced mobility, similar to that found at grain boundaries. If true, this would be of considerable importance in with regards to the devitrification process.